Cmfit

software for analysis of waveforms sampled by digitizers in semi-digital mode

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1. Introduction

The software described here was developed for digital measurement of Doppler broadening in so called semi-digital mode [1-3]. Our code performs analysis of pulses from high purity Ge (HPGe) detectors shaped by pseudo-Gaussian filter in spectroscopy amplifiers and sampled by digitizers.

- **Cmfit** – code is the main program for analysis of sampled waveforms. It performs energy calibration, eliminates pulses with distorted shape using digital filters and creates 1D and 2D gamma ray energy spectra
- **cDCDB gen** – utility which generates synthetic data for testing purposes. These data can be used to check proper functionality of cmfit code.

The users are however kindly requested to cite the use of our codes in their works using the reference J. Čížek. M. Vlček, I. Procházka, Nuclear Instruments and Methods in Physics Research Section A, 623, 982-994 (2010).

2. Source code and building of executables

The programs Cmfit and cDCDB gen are written in C++. The source code can be downloaded from the web page http://physics.mff.cuni.cz/kfnt/pas/?page=software.

3. Function of the programs

The analysis of sampled waveforms by Cmfit code is performed in a series of sequential runs called *modes*. The following modes are available:

- `mode = -1`: diagnostic mode used to visualize waveforms and set the parameters required for further analysis
- `mode = 0`: raw selection of data using so called *fixed filters*, energy calibration and digital *shape filters* are created
- `mode = 1`: single energy spectra for both detectors are created, fine selection of data by *shape filters*
- `mode = 2`: 1D and 2D energy spectra of coincidence gamma rays are created, only raw selection of waveforms is performed using *fixed filters*
- `mode = 3`: 1D and 2D energy spectra of coincidence gamma rays are created, fine selection of waveforms is performed by *shape filters*

When the Cmfit code is started it firstly looks for the input files `calibration.ini`, `cmfit.ini`, `histograms.ini`, `suffix.ini`, and `watchdogs.ini`. These files should be located in the directory where the program is started. Subsequently the program reads the waveform from data files and performs the analysis. Results are written to various output files created by the program. Output files are written to the working directory where the Cmfit program was started and any old output files existing in this folder are overwritten. Therefore it is recommended to create a new directory for each mode.

4. Data files

A point sampled by digitizer is called a *sample*. Digitized pulse consisting of certain number of samples (specified in the input file `cmfit.ini`) is called *waveform*. Acquisition is performed in parts called *sessions*. The number of waveforms per session is again specified in the input file `cmfit.ini`. Waveforms collected in each session are stored in separate file.
Cmfit code expects that sampled data are stored in binary files created by the acquisition programs Dacqn and cDacqn. The data files have to be named `name-`*`n`*`.Suffix`, where *n* is the current number of session, `name` is a descriptor of spectrum specified by user and `Suffix` is string which identifies data acquired in single and in coincidence mode. Suffixes are specified by user in the input file section `suffix.ini`.
The binary data files are expected to have the following structure:
`Samples, Segments, Waveforms, w1_ch1[1], w1_ch2[1], ... , w2_ch1[1], w2_ch[1], ......,` i.e. each file begins with three integers (32-bits) `Samples, Segments, Waveforms` representing the number of samples per waveform, the number waveforms per segment and the number of waveforms per session; a list of short integers (16-bits) `w1_ch1[1], w1_ch2[1], ...` representing the first sample of the first waveform in the channel 1 (`w1_ch1[1]`), the first sample of the first waveform in the channel 2 (`w1_ch2[1]`), the second sample of the first waveform in the channel 1 (`w1_ch1[2]`), the second sample of the first waveform in the channel 2 (`w1_ch1[2]`), etc `...` the first waveform is followed by the second waveform `w2_ch1[1], w2_ch2[1], ...` and next waveforms in the same manner.

5. Input files

The input files `calibration.ini`, `cmfit.ini`, `histograms.ini`, `suffix.ini`, and `watchdogs.ini` must be located in the directory where the program Cmfit is started.
The input files are ASCII files with the following structure: each entry must be on a separate line. There must not be blank lines between various entries. Each line starts with a `parameter`, i.e. a number or numbers separated by coma or a string. Any text after `parameter` up to the end of line (`'\n'`) is considered as a comment and is ignored. The easiest way how to prepare the input file is to edit the templates supplied with the source codes. The Cmfit code writes the `parameters` read from the input files on the screen which enables user to check if the input files were read correctly. In the following text the meaning of all entries in the input files is explained.

`Cmfit.ini`

This is the main input file driving the run of Cmfit code. An example of the input file `cmfit.ini` with explanation of all entries is given in the following text

```
0  !mode (line 1)
```

Switch which species the running mode of the Cmfit code. The following modes are available `mode = -1`: diagnostic mode used to visualize waveforms and set the parameters required for further analysis. Waveforms sampled in channel 1 and channel 2 are written to textual files `wav1.txt` and `wav2.txt` in a two-column x y format. The derivatives of the waveforms are written to files `wdif1.txt` and `wdif2.txt`. Number of waveforms written to these files is specified by the `number of waveforms` switch and should not be too

high since it would make the textual files very large. Typically only a few waveforms are analyzed in mode -1 in order to check shape of typical pulse.
`mode = 0`: This is basic mode which must be run prior to modes 1, 2, 4. In the mode 0 the baseline position is determined and written to the output file `stability.txt`, the energy calibration is created and written to the output file `e-cal.txt`. The ideal pulse shape and upper and lower bound for shape filters are determined and written to the output file `peakm.txt`. Raw selection of data using *fixed filters* is performed.
`mode = 1`: In addition to the input files, the output files `stability.txt`, `e-cal.txt`. and `peakm.txt` created in the mode 0 must be located in the working directory. Single energy spectra for both detectors are created, fine selection of data is performed by *shape filters*.
`mode = 2`: In addition to the input files, the output files `stability.txt`, `e-cal.txt`. and `peakm.txt` created in the mode 0 must be located in the working directory. 1D and 2D energy spectra of coincidence gamma rays are created, only raw selection of waveforms is performed using *fixed filters*
`mode = 3`: In addition to the input files, the output files `stability.txt`, `e-cal.txt`. and `peakm.txt` created in the mode 0 must be located in the working directory. 1D and 2D energy spectra of coincidence gamma rays are created, fine selection of waveforms is performed by *shape filters*

```
1000       !number of samples (line 2)
```
This entry specifies the number of samples per waveform in the data file

```
100000     !number of waveforms (line 3)
```
This entry specifies the number of waveforms per session, i.e. the number of waveforms in each data file

```
1          !number of sessions (line 4)
```
The number of sessions which have to be analyzed.

```
c:\bulk\dcdb\synth\synth  !(line 5)
```
Path to the data files.

```
0     !calibration 0-average, 1-independent, 2-smoothed (line 6)
```
A switch for energy calibration
0 – energy calibration calculated as average over the whole measurement is used.
1 – energy calibration is performed independently for each session
2 – energy calibration is performed independently for each session used smoothed data

```
500,500    !reference point ch1,ch2  (line 7)
```
Reference point on the horizontal axis in channel 1 and channel 2 to which the position of maximum of a waveform is shifted when the waveform is normalized.

```
5,5        !waveform smoothing (line 8)
```
Number of samples which will be averaged (size of moving average window) to smooth the sampled waveforms.

```
0.25,0.25   !wdif_threshold (line 9)
```
Threshold applied on the derivative of waveform to determine the onset of the pulse in channel 1 and channel 2.

```
20,40          !wdif smoothing (line 10)
```
Number of samples which will be averaged (size of moving average window) to smooth the derivative of waveform.

```
16             !raw divider  12-bit digitizer 16 (line 11)
```
Number by which the raw samples created by digitizer are divided to get integers. For 12-bit digitizer it is 16.

```
100            !shift offset (line 12)
```
Maximum acceptable value of shift of the peak maximum bin to the reference point. It specifies also number of channels from the beginning and the end of the waveform which are not used in the analysis, see Fig. 1 for a graphical explanation.

```
50             !wmax fit range (line 13)
```
The range (in bins) around peak maximum which will be used for parabolic fitting of maximum, see Fig. 1.

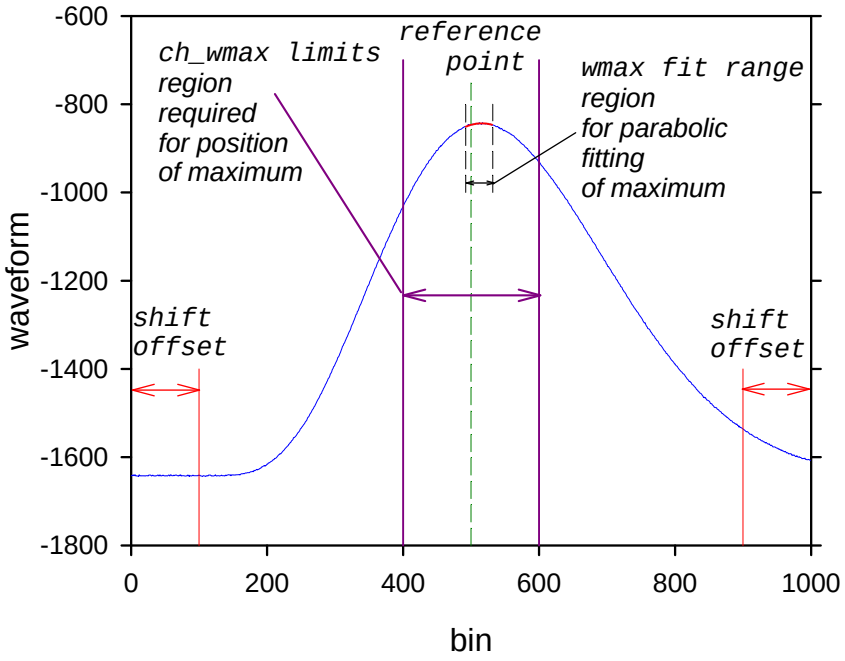

Fig. 1 *An example of a single waveform with description of the parameters specified by the user in the input files cmfit.ini a watchdogs.ini.*

```
2,2            !delta for cuts RF,DB (keV) (line 14)
```
Width of the bands (in keV) for vertical and horizontal cuts from 2D energy spectrum created in modes 2,4, see Fig. 6.

```
-30,30         !RF histogram range (keV) (line 15)
```
Range of the vertical scale $E_1 + E_2 - 2m_0c^2$ (in keV) for 2D energy spectrum created in modes 2,3, see Fig. 6.

```
-30,30         !DB histogram range (keV) (line 16)
```
Range of the horizontal scale E_1 - E_2 (in keV) for 2D energy spectrum created in modes 2,3, see Fig. 6.

`-1000,1000  !aif histogram range (line 17)`
Range of histogram for the annihilation-in-flight contribution

`2.0,2.0     !f_ext_l f_ext_r (line 18)`
Extension factors (left and right) of shape filters.

`0           !textual mode 0-quiet 1-verbose (line 19)`
This entry specifies how detailed the textual output of the program should be.

`Watchdogs.ini`

This is input file which specifies so called fixed filters, i.e. filters used for a raw selection of waveforms and rejection of seriously damaged pulses. There are four watchdogs which can be applied for inspection of waveforms:
1. *check of the maximum* of the pulse – this watchdog is used to reject pulses so large that maximum of the vertical scale of digitizer was exceeded.
2. *check of the position of maximum* of the pulse – this watchdog check if the maximum of the pulses fall into pre-selected range around the reference point given is the entry `reference point` in cmfit.ini. Since maximum of each pulse is shifted to the reference point when digital filters are created it is important to select the region required for position of maximum so that the distance between the lower limit and the reference point does not exceed `shift offset` given in `cmfit.ini`. Similarly the distance between the reference point and the upper limit should not exceed the `shift offset`, see also Fig. 1.
3. χ^2 *test of parabolic fit of pulse maximum* – this watchdog makes χ^2 *test* of the parabolic fit of pulse maximum. It the parabolic is not good enough, i.e. the pulse is rejected if it does not have well defined maximum which can be described by parabolic shape.
4. *test of rms of baseline* – this watchdog calculates *rms* of baseline prior to the pulse. If baseline is too noisy the pulse is rejected.
Each watchdog can be switched on by setting its switch in `watchdog.ini` to `1` or it can be switched off by setting the switch to `0`. `Watchdog.ini` has the following structure:

`0            !wf maximum watchdog (line 1)`
This is switch for the first watchdog which checks maximum of the pulse. Now it is switched off.

`-1625,2000   !wmax1 limits (line 2)`
Allowed range into which the maximum of the pulse from the first detector has to fall. If it falls outside this range the pulse will be rejected.

`-1625,2000   !wmax2 limits  (line 3)`
Allowed range for the maxima of pulses from second detector

`1            !wf channel of maximum watchdog  (line 4)`
Switch for the second watchdog which checks position of maximum of the pulse. Now it is switched on.

`400,600      !ch_wmax1 limits`
Allowed range for the position of maximum of the pulse from the first detector. If it falls outside this range the pulse will be rejected. Note that this range should selected so that

distance between the lower limit and the `reference point` does not exceed `shift offset` specified in `cmit.ini`. Similarly the distance between the upper limit and the `reference point` should not exceed `shift offset.`

```
500,700         !ch_wmax2 limits (line 5)
```
Allowed range for the position of maximum of the pulse from the second detector.

```
0                !chi2 parabolic fit of maximum watchdog (line 6)
```
Switch for the third watchdog which examines quality parabolic fit of pulse maximum by χ^2 test. Now it is switched off

```
10,250          !chi2sq1 limits (line 7)
```
Allowed range for χ^2 values for pulses from the first detector. If χ^2 value for a pulse falls outside this range the pulse will be rejected.

```
10,250          !chi2sq2 limits (line 8)
```
Allowed range for χ^2 values for pulses from the second detector.

```
0               !rms of baseline watchdog (line 9)
```
Switch for the third watchdog which checks *rms* of the baseline Now it is switched off

```
5,250           !bcg_sigma1_l limits (line 10)
```
Allowed range for *rms* values for pulses from the first detector. If *rms* value for a pulse falls outside this range the pulse will be rejected.

```
5,250           !bcg_sigma2_l limits (line 11)
```
Allowed range for *rms* values for pulses from the second detector.

`Calibration.ini`

This is input file for energy calibration of spectra from both detectors. The calibration procedure finds maximum in the energy spectrum in range selected by user. For energy calibration two peaks with known energies are necessary.
First line of Calibration.ini contains range (in samples) where the first peak (peak1) should be located in the spectrum measured by the first detector, e.g. the entry

```
600,1000   !bdif1 peak1 raw range
```
means that first peak (peak1) is located between the channel 600 and 1000. Second line gives the range for the peak1 in the spectrum for the second detector. Third line specifies the range where the second peak (peak2) is located in the spectrum from the first detector and fourth line specifies this range for the second detector.
Finally the last line gives the known energies (in keV) and the peak1 and peak2.
Note:
If only one peak is available in the spectrum. One can use calibration with energy 0 keV at channel 0. This can be done by setting the energy range for the peak1 (line1 and line2) 0,0 and the energy of the peak1 in the last line 0.

Example of `calibration.ini`:

```
600,1000   !bdif1 peak1 raw range
600,1000   !bdif2 peak1 raw range
1400,1900  !bdif1 peak2 peak raw range
```

```
1400,1900  !bdif2 peak2 raw range
511,1078   !energies for calibration peak1, peak 2
```

Here the peak1 has energy of 511 keV (annihilation peak) and is located between the channel 600 and 1000 in the spectra of both detectors. Second peak (peak2) has energy 1078 keV, i.e. (^{68}Ge/^{68}Ga) secondary γ-ray, and is located between the channel 1400 and 1900 in the spectra of both detectors.

Another example of `calibration.ini`:

```
0,0      !bdif1 peak1 raw range
0,0      !bdif2 peak1 raw range
400,900  !bdif1 peak2 peak raw range
300,500  !bdif2 peak2 raw range
0,511    !energies for calibration peak1, peak 2
```

Here the calibration is made so that zero energy is in the zero channel for both detectors. Only one peak with energy of 511 keV, i.e. the annihilation peak, is used for calibration. This peak is located between the channel 400 and 900 in the spectra of the first detector and between the channel 300 and 500 in the spectra of the second detector.

The ranges corresponding to various peaks can be found using histograms in the file `hist-bdif.txt`, which contain non-calibrated energy spectrum of both detectors, see Fig. 5.

`Suffix.ini`

This is input file specifies suffixes of data files analyzed in various modes. `Suffix.ini` has the following structure:

`cdb  !mode -1 (line 1)`

The suffix (3 characters) of the data files analyzed in the mode -1. Here the suffix is `cdb`. Hence the data files are expected to be named `xxxxx-1.cdb`, `xxxxx-2.cdb`, etc., where `xxxxx` is the generic name of the measurement.

Note that if the suffix is specified as `*` then the programs expects data files to be named `xxxxx.1`, `xxxxx.2`, etc., where `xxxxx` is the generic name of the measurement.

`sgl  !mode 0 (line 2)`

The suffix of the data files analyzed in the mode 0. Here the suffix is `sgl`. Hence the data files are expected to be named `xxxxx-1.sgl`, `xxxxx-2.sgl`, etc., where `xxxxx` is the generic name of the measurement.

`sgl  !mode 1 (line 3)`

The suffix of the data files analyzed in the mode 1.

`cdb  !mode 2 (line 4)`

The suffix of the data files analyzed in the mode 2.

`cdb  !mode 3 (line 5)`

The suffix of the data files analyzed in the mode 3.

Histograms.ini

This is input file which specifies ranges of histograms created by cmfit. Every line of `Histograms.ini` contains range, i.e. lower limit and upper limit of some histogram which will be created during analysis of data. Specification of histograms is given the following text

```
0,1350    !bdif1_cal - energy spectrum detector 1 (line 1)
```

Calibrated energy spectrum for detector 1. The limits are given in keV. The histogram is written into the file `hist-bdif-cal.txt`.

```
0,1350    !bdif2_cal - energy spectrum detector 2 (line 2)
```

Calibrated energy spectrum for detector 2. The limits are given in keV. The histogram is written into the file `hist-bdif-cal.txt`.

```
0,1e4     !darea1 (line 3)
```

Energy spectrum (non-calibrated) created from areas of pulses for detector 1. The histogram is written into the file `hist-darea.txt`.

```
0,1e4     !darea2 (line 4)
```

Energy spectrum (non-calibrated) created from areas of pulses for detector 2. The histogram is written into the file `hist-darea.txt`.

```
0,1e7     !warea1 (line 5)
```

Spectrum created from positive areas of waveform derivatives of pulses for detector 1. The histogram is written into the file `hist-warea.txt`.

```
0,1e7     !warea2 (line 6)
```

Spectrum created from positive areas of waveform derivatives of pulses for detector 2. The histogram is written into the file `hist-warea.txt`.

```
-2000,-1250   !bcg1_mean_l (line 7)
```

Histogram of baseline levels of pulses for detector 1. The histogram is written into the file `hist-bcg_mean.txt`.

```
-2000,-1250   !bcg2_mean_l (line 8)
```

Histogram of baseline levels of pulses for detector 2. The histogram is written into the file `hist-bcg_mean.txt`.

```
0,500         !bcg1_sigma_l (line 9)
```

Histogram of rms of baseline of pulses for detector 1. The histogram is written into the file `hist-bcg_sigma.txt`.

```
0,500         !bcg2_sigma_l (line 10)
```

Histogram of rms of baseline of pulses for detector 2. The histogram is written into the file `hist-bcg_sigma.txt`.

```
0,4096        !bdif1 histogram range (line 11)
```

Non-calibrated energy spectrum for detector 1. The histogram is written into the file `hist-bdif.txt`.

```
0,4096        !bdif2 histogram range (line 12)
```

Non-calibrated energy spectrum for detector 2. The histogram is written into the file `hist-bdif.txt`.

`-2048,2048    !wmax1 histogram range (line 13)`
Histogram of maxima of waveform derivatives for detector 1. The histogram is written into the file `hist-wmax.txt`.

`-2048,2048    !wmax2 histogram range (line 14)`
Histogram of maxima of waveform derivatives for detector 2. The histogram is written into the file `hist-wmax.txt`.

`0,1000        !ch_wmax1 histogram range (line 15)`
Histogram of positions of maxima of waveform derivatives for detector 1. The histogram is written into the file `hist-ch_wmax.txt`.

`0,1000        !ch_wmax2 histogram range (line 16)`
Histogram of positions of maxima of waveform derivatives for detector 2. The histogram is written into the file `hist-ch_wmax.txt`.

`0,50         !chi2sq1 histogram range (line 17)`
Histogram of χ^2 values obtained for parabolic fit of maxima of pulses for detector 1. The histogram is written into the file `hist-chi2sq.txt`.

`0,50         !chi2sq2 histogram range (line 18)`
Histogram of χ^2 values obtained for parabolic fit of maxima of pulses for detector 2. The histogram is written into the file `hist-chi2sq.txt`.

`0,500         !ch_darea1 histogram range (line 19)`
Histogram of centroids of pulses for detector 1. The histogram is written into the file `hist-ch_darea.txt`.

`0,500         !ch_darea2 histogram range (line 20)`
Histogram of centroids of pulses for detector 2. The histogram is written into the file `hist-ch_darea.txt`.

`0,1000        !t1 histogram range (line 21)`
Histogram of times of appearance of pulses for detector 1. The histogram is written into the file `hist-t.txt`.

`0,1000        !t2 histogram range (line 22)`
Histogram of times of appearance of pulses for detector 2. The histogram is written into the file `hist-t.txt`.

`-500,500      !dt histogram range (line 23)`
Histogram of time differences between pulses from detector 1 and detector 2. The histogram is written into the file `hist-dt.txt`.

`400,500,600   !channels for cuts in fpeakh (line 24)`

Channels where one-dimensional cuts from two-dimensional histogram pulse shapes will be made. These one-dimensional cuts will be written to the file `fpeakh.txt`.

Note that the most important histograms are `bdif` and `bdif_cal` containing non-calibrated and calibrated energy spectra for both detectors.

6. A complete example of analysis

An example of complete analysis of acquired waveforms is described in the following text. The waveforms were measured using two HPGe detectotrs, ^{68}Ge/^{68}Ga positron generator and pure Mg target.
As a result of analysis in all modes the program creates a number of histograms. Histogram files have standard designation `hist-xxxxx.txt`, where the string `xxxxx` is the name of histogram. The structure of histogram files is as follows:
`i x1[i] y1[1] x2[i] y2[i],`
Where `i` is the increamenting index, `x1[i]` (float) is the position of *i*-th bin of the histogram and `y1[i]` (integer) is the number of counts in *i*-th bin of the histogram for the first detector. Simlarly `x2[i]` (float) and `y2[i]` (integer) are the position of *i*-th bin and the number of counts in *i*-th bin for the second detector.
In addition the program always creates protocol file `cmfit.log` containing information about all settings read from the input files, names of all data files analyzed and summary with statistics of the fraction of good waveforms.

6.1. Setting of parameters (mode = -1)

Required input files:
`calibration.ini`
`cmfit.ini`
`histograms.ini`
`suffix.ini`
`watchdogs.ini`

Created output files:
files with acquired pulses:
`swav1.txt, swav2.txt`
`wdif1.txt, wdif2.txt`
`parabola1.txt, parabola2.txt`
histograms:
`hist-bcg_mean.txt`
`hist-bcg_sigma.txt`
`hist-bdif.txt`
`hist-bdif-sess.txt`
`hist-ch_darea.txt`
`hist-ch_wmax.txt`
`hist-chi2sq.txt`
`hist-darea.txt`
`hist-dt.txt`
`hist-t.txt`
`hist-warea.txt`
`hist-wmax.txt`

Firstly one should run cmfit in diagnostic mode (mode = -1) to examine how the acquired waveforms look like. In this mode that program creates output files `swav1.txt`, `swav2.txt` containing waveforms and files `wdif1.txt` and `wdif2.txt` containing waveform derivatives.

The file `swav1.txt` contains 4 columns:

`ch[i][j] w[i][j] sw[i][j] sw[i][j]-w[i][j]`,

where `ch[i][j](integer)` is the *i*-th bin of *j*-th waveform, `w[i][j](integer)` is the *i*-th point of *j*-th waveform and `w[i][j](float)` is the *i*-th point of *j*-th waveform smoothed using smoothing factor specified in the entry `waveform smoothing (line 8)` in `cmfit.ini`. Individual waveforms are separated by a blank line. The file `swav2.txt` contains analogical data for the second detector. Fig. 1 shows an example of 100 waveforms measured by one and second detector.

The file `wdif1.txt` contains 4 columns:

`ch[i][j] wd[i][j] swd[i][j] swd[i][j]-wd[i][j]`,

where `ch[i][j](integer)` is the *i*-th bin of *j*-th the waveform derivative, `w[i][j](integer)` is the *i*-th point of *j*-th waveform derivative and `w[i][j](float)` is the *i*-th point of *j*-th waveform derivative smoothed using the smoothing factor specified in the entry `wdif smoothing (line 10)` in `cmfit.ini`.

The number of waveforms written into files `swav1.txt`, `swav2.txt` and `wdif1.txt` and `wdif2.txt` is specified in the input file `cmfit.ini` by the entries `number of waveforms (line 3)` and `number of sessions (line 4)`.

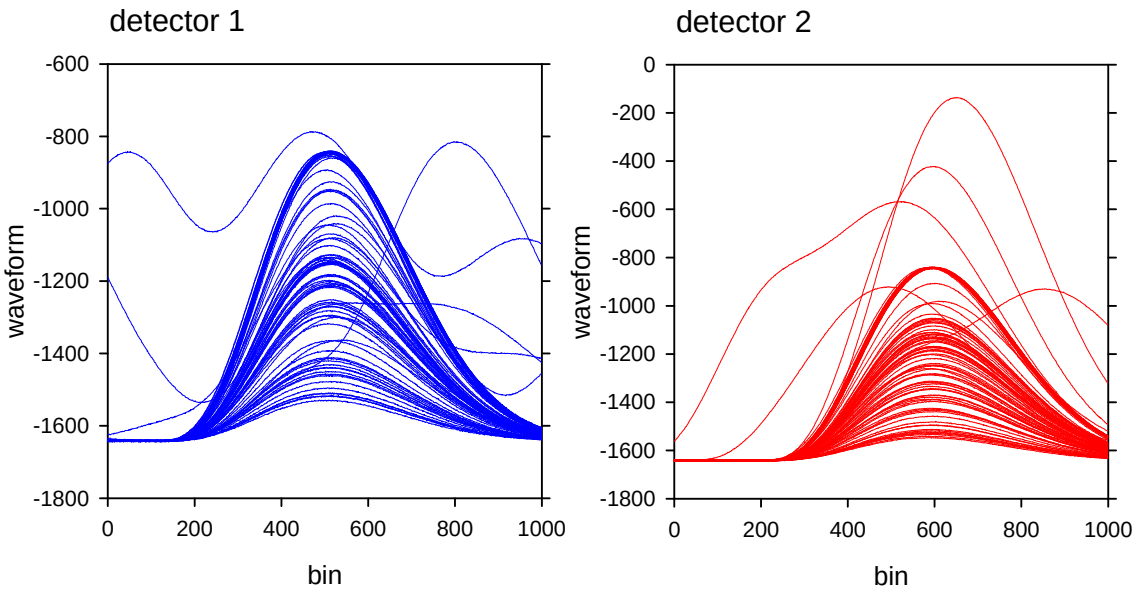

Fig. 1 *An example of 100 sampled waveforms from one and second detector. The waveforms were read from the file swav1.txt and swav2.txt created in mode -1.*

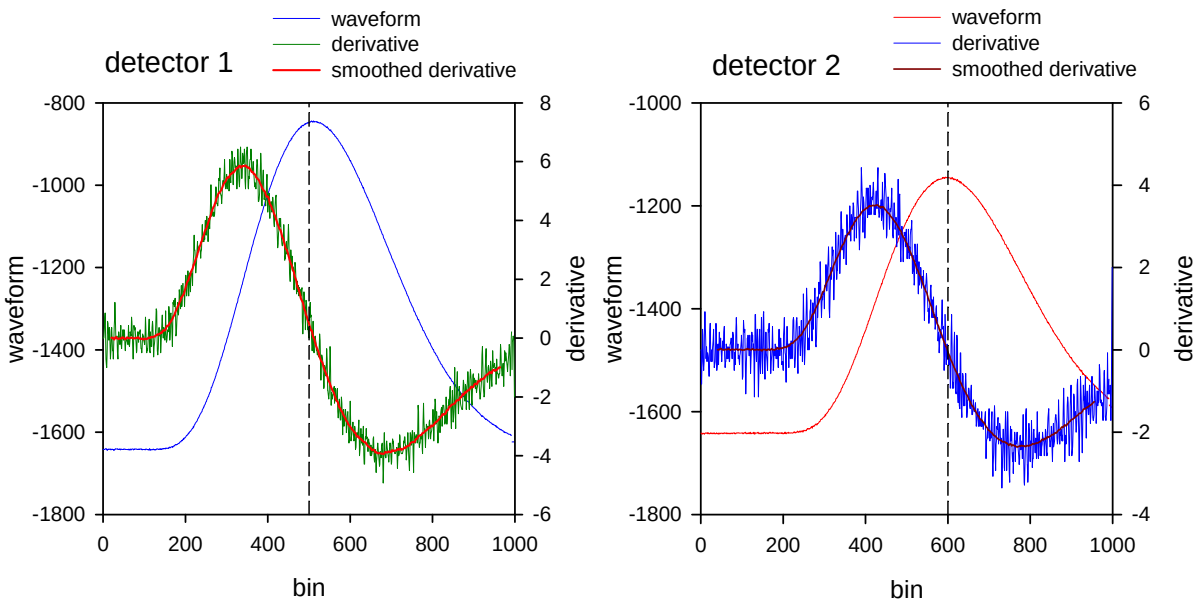

Fig. 2 *An example of a single waveform, its derivative and smoothed derivative. The waveforms were read from the files swav1.txt and swav2.txt, the derivatives were read from the files wdif1.txt, wdif2.txt created in mode -1. The dashed lines show position of the selected refence point.*

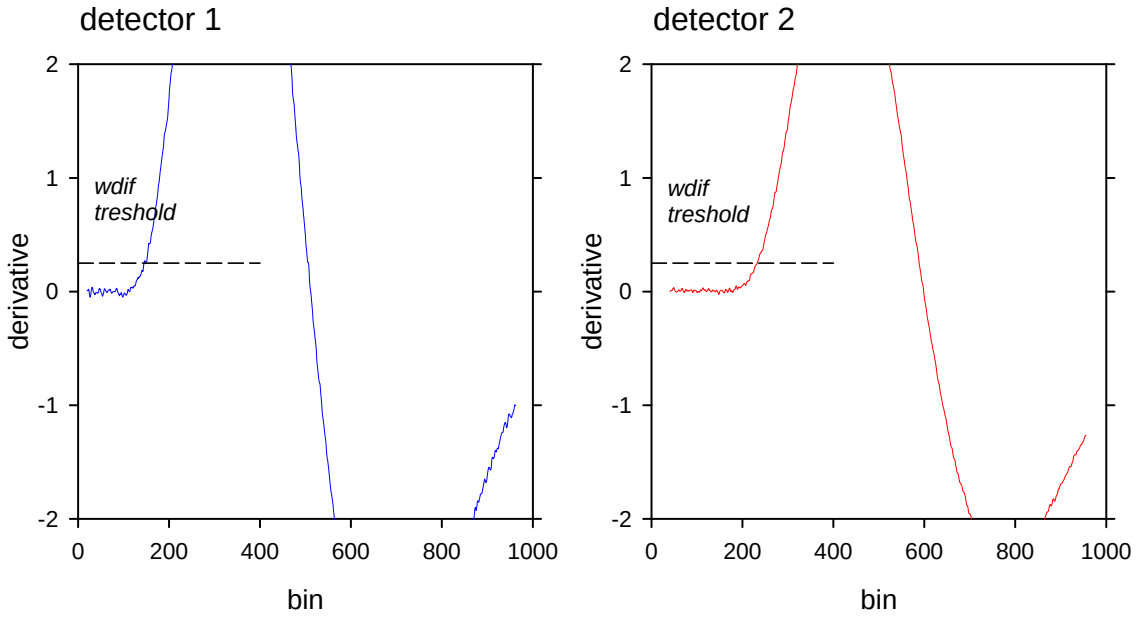

Fig. 3 *Smoothed derivative of a randomly selected single waveform. Dashed line shows position of treshold applied on the derivative of waveform to determine the onset of the*

Notes:

1. That number of waveforms recorded in mode -1 should not be too high otherwise the files `swav1.txt`, `swav2.txt` and `wdif1.txt` and `wdif2.txt` become very large. Typically it is sufficient to record ~ 100 waveform for examination.
2. No filtering of waveforms is performed, i.e. every acquired waveform is written into the files `swav1.txt`, `swav2.txt`. One can see in Fig. 1 that that there are obviously some waveforms with shape distorted by pile-ups.

A single randomly selected waveform for each detector is plotted in Fig. 2 together with its rough derivative `wd[i][j]` and smoothed derivative `swd[i][j]` (both taken from files `wdif1.txt` and `wdif2.txt`). Such pot can be used to chose parameters of smoothing of waveform derivatives; here 20 and 40 channels for the first and the second detector, respectively. The dashed lines in Fig. 2 show position of the reference points for the first and the second detector selected by user in the entry `reference point ch1,ch2 (line 7)` in `cmfit.ini`. Reference point is the channel to which the position of maximum of each waveform is shifted when the waveform is normalized and should be selected close to the channel where maxima of waveforms are typically reached. In this example reference points 500 and 600 were selected for the first and the second detector.
Maxima of waveforms are determined by parabolic fitting in the region around the channel with maximum value of the waveform. The width of the region where parabolic fitting will be performed is specified by the entry `wmax fit range` in `cmifit.ini`. Here in this example it was 50 bins. To select the width of the fitting region one can use output files `parabola1.txt` and `parabola2.txt` containing parabolic fits for analyzed waveforms. In Fig. 4 the parabolic fits taken from files `parabola1.txt` and `parabola2.txt` are plotted together with the waveforms obtained from files `swav1.txt` and `swav2.txt`.

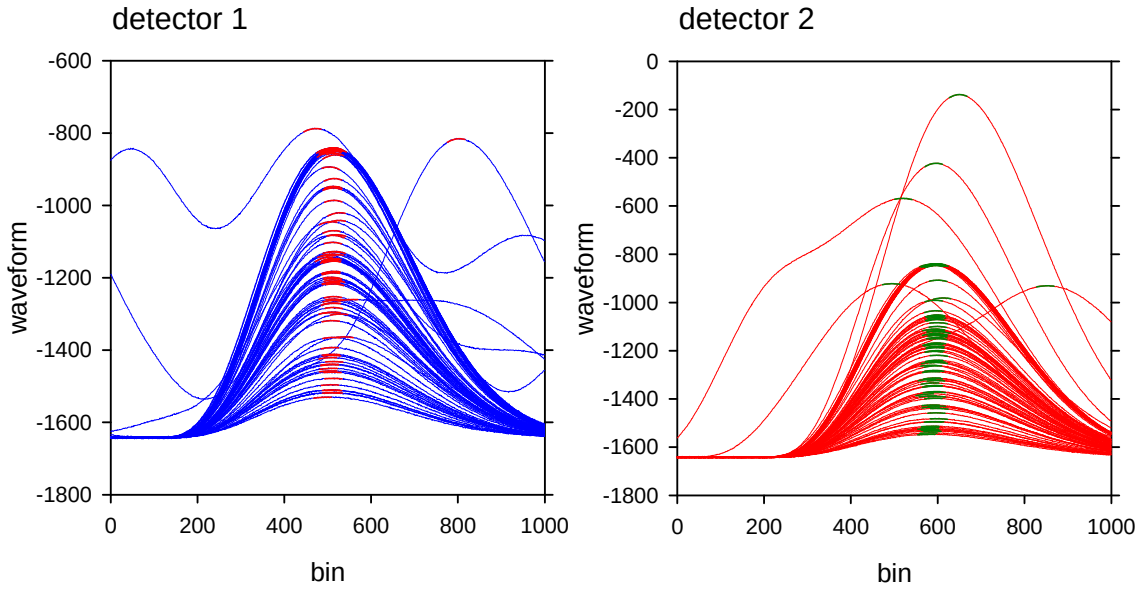

Fig. 4 *An example of 100 sampled waveforms from one and second detector together with parabolic fits of the regions around maxima. The waveforms were read from the file swav1.txt and swav2.txt and the parabolic fits were taken from files parabola1 and parabola2 created in the mode -1.*

The summary of adjustment of the parameters in `cmit.ini` after analysis in mode -1:

```
-1          !mode
1000        !number of points
100         !number of waveforms
1           !number of sessions
h:\mggn2\mggn2  !name of the spectrum in this example
1            !calibration
500,600      !reference point ch1,ch2
```

```
5,5          !waveform smoothing
0.5,0.5      !wdif_treshold
20,40        !wdif smoothing
16           !raw divider  12-bit digitizer 16
100          !shift offset
50           !wmax fit range
2,2          !delta for cuts RF,DB (keV)
-30,30       !RF histogram range (keV)
-30,30       !DB histogram range (keV)
2.0,2.0      !f_ext_l f_ext_r
1            !textual mode 0-quiet 1-verbose
```

6.2. Raw analysis of waveforms (mode = 0)

Required input files:

```
calibration.ini
cmfit.ini
histograms.ini
suffix.ini
watchdogs.ini
```

Created output files:

histograms:

```
hist-bcg_mean.txt
hist-bcg_sigma.txt
hist-bdif.txt
hist-bdif-sess.txt
hist-ch_darea.txt
hist-ch_wmax.txt
hist-chi2sq.txt
hist-darea.txt
hist-dt.txt
hist-t.txt
hist-warea.txt
hist-wmax.txt
```

files for calibration and examination of stability:

```
e-cal.txt
e-cal-smooth.txt
stability.txt
```

file with ideal pulse shape and shape filters:

```
peakm.txt
```

As a second step cmfit is run in the raw analysis mode (mode = 0). The aim of this mode is

- to create non-calibrated energy spectra from both detectors
- examine stability of the system
- create shape filters

non-calibrated energy spectra

In mode 0 the waveforms are processed in the standard way but only fixed filters specified in the input file `watchdogs.ini` are applied for raw selection of waveforms, i.e. to reject seriously distorted waveforms.

Energy of detected γ-ray is determined as height of the pulse, i.e. the difference between the pulse maximum determined by parabolic fitting performed in the range specified by the entry `wmax fit range` in `cmifit.ini` and the baseline. The non-calibrated energy spectra for both detectors are stored in the histogram file `hist-bdif.txt` and are plotted in Fig. 5.

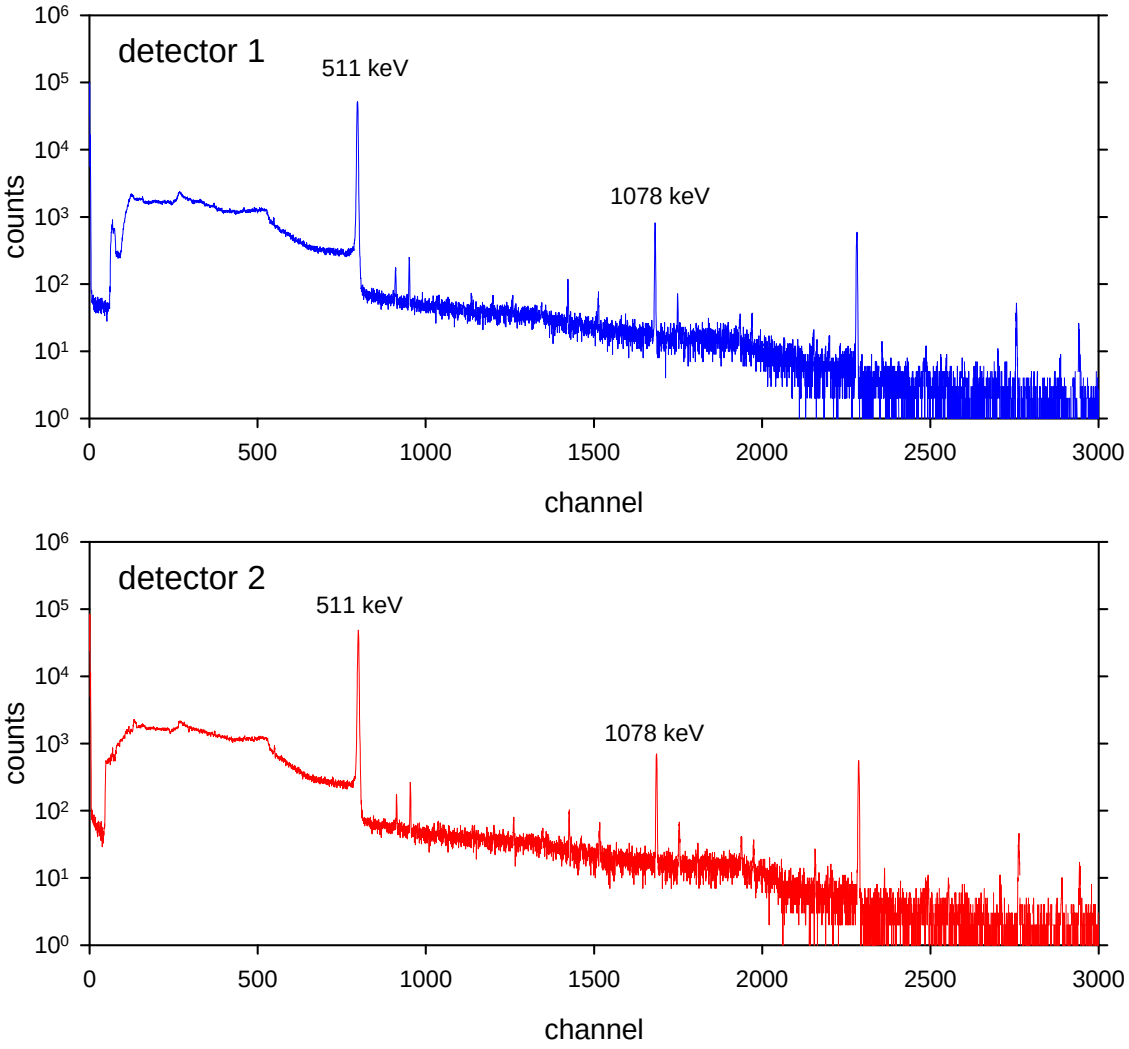

Fig. 5 *Non-calibrated energy spectra measured with $^{68}Ge/^{68}Ga$ source in the single mode. The spectra were taken from the histogram hist-bdif.txt created in the mode 0.*

stability of the system

Digital measurement is performed in portions called sessions. This enables to examine and correct walk of the baseline and changes of gain of detector preamplifiers and spectroscopy amplifiers. Positions of baseline and both calibration peaks are determined independently in each session and written into the output file `e-cal.txt`. The file `e-cal.txt` consists of 11 columns and has the following structure

`i baseline_d1[i] peak1_d1[i] FWHM1_d1[i] peak2_d1[i] FWHM_d1[i] baseline_d2[i] peak1_d2[i] FWHM1_d2[i] peak2_d2[i] FWHM_d2[i]`, where `i` is the number of session, `baseline_d1[i]` is the position of baseline in the *i*-th session for the first detector, `peak1_d1[i]` and `FWHM1_d1[i]`are position and FWHM of peak1 for the first detector and `peak2_d1[i]` and `FWHM2_d1[i]`are position and FWHM of peak2 for the first detector; `baseline_d2[i] peak1_d2[i] FWHM1_d2[i] peak2_d2[i] FWHM_d2[i]` are the same quantities for the second detector. Fig. 5 shows the development of position of baseline and positions of peak1 and peak2 for the first detector in various sessions. The file `e-cal.txt` is used for *independent* energy calibration in modes 1,2,3 specified by switch 1 in the entry `calibration` in `cmfit.ini`. Smoothed developments of quantities in the file `e-cal.txt` are stored in the output file `e-cal-smooth.txt` and this file is used for *smoothed independent* energy calibration specified by switch 2 in the entry `calibration` in `cmfit.ini`.

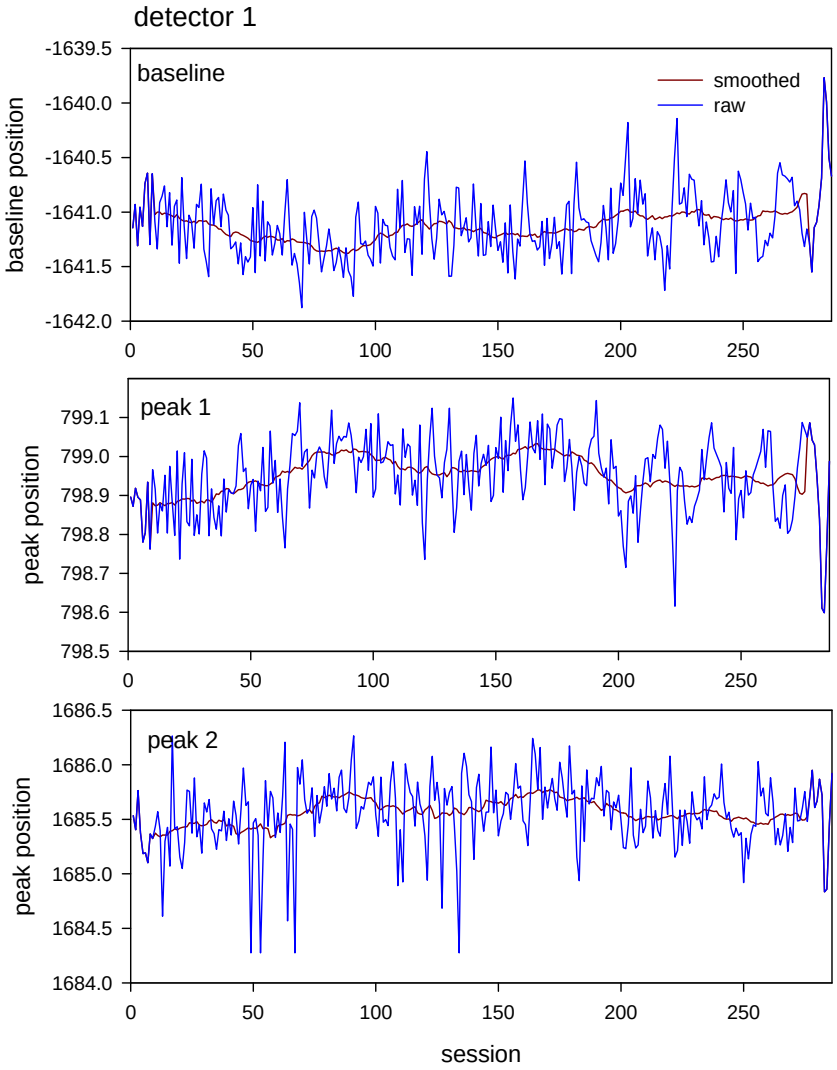

Fig. 6 *An example development of baseline position and positions of the peak 1 and peak 2 for detector 1. The data were taken from file e-cal.txt (raw data) and e-cal-smooth.txt (smoothed curve).*

The development of baseline position and positions of peak 1 and peak 2 for detector 1 taken from the output file `e-cal.txt` are plotted in Fig. 5 together with the smoothed curves taken form output file `e-cal-smooth.txt`. Note that baseline position and FWHM of the peak 1 and peak 2 for both detectors are written also to the output file `stability.txt`.

creation of shape filters
In the analysis the waveforms are normalized and shifted to the predefined reference point. The ideal shape of waveform is determined from the normalized waveforms as modus, i.e. the most probable value in each channel. The lower and bound around the ideal shape of waveform is determined at the points where the distribution in given channel falls to one tenth of the maximum value. The ideal shapes of waveform together with the lower and the upper bound for both detectors are stored in the file `peakm.txt`. The ideal shape of waveform and upper and lower bound for the first detector are plotted in Fig. 5.

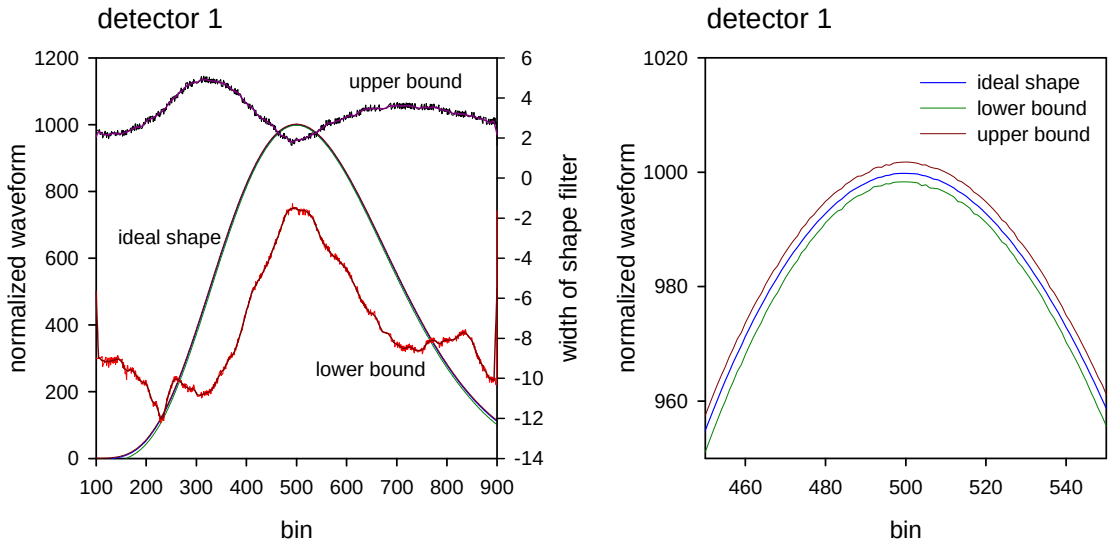

Fig. 7 *Left panel: the ideal shape of waveform and lower and upper bound bound (calculated and smoothed curve); right panel: detail around maximum of waveform with lower and upper bound.*

6.3. Fine analysis of waveforms (mode = 1)

Required input files:
`calibration.ini`
`cmfit.ini`
`histograms.ini`
`suffix.ini`
`watchdogs.ini`
calibration files created in mode 0:
`e-cal.txt`
`e-cal-smooth.txt`
file with ideal pulse shapes and shape filters created in mode 0:
`peakm.txt`

Created output files:
histograms:

```
hist-bcg_mean.txt
hist-bcg_sigma.txt
hist-bdif.txt
hist-bdif-cal.txt
hist-bdif-sess.txt
hist-ch_darea.txt
hist-ch_wmax.txt
hist-chi2sq.txt
hist-darea.txt
hist-dt.txt
hist-reject.txt
hist-t.txt
hist-warea.txt
hist-wmax.txt
```

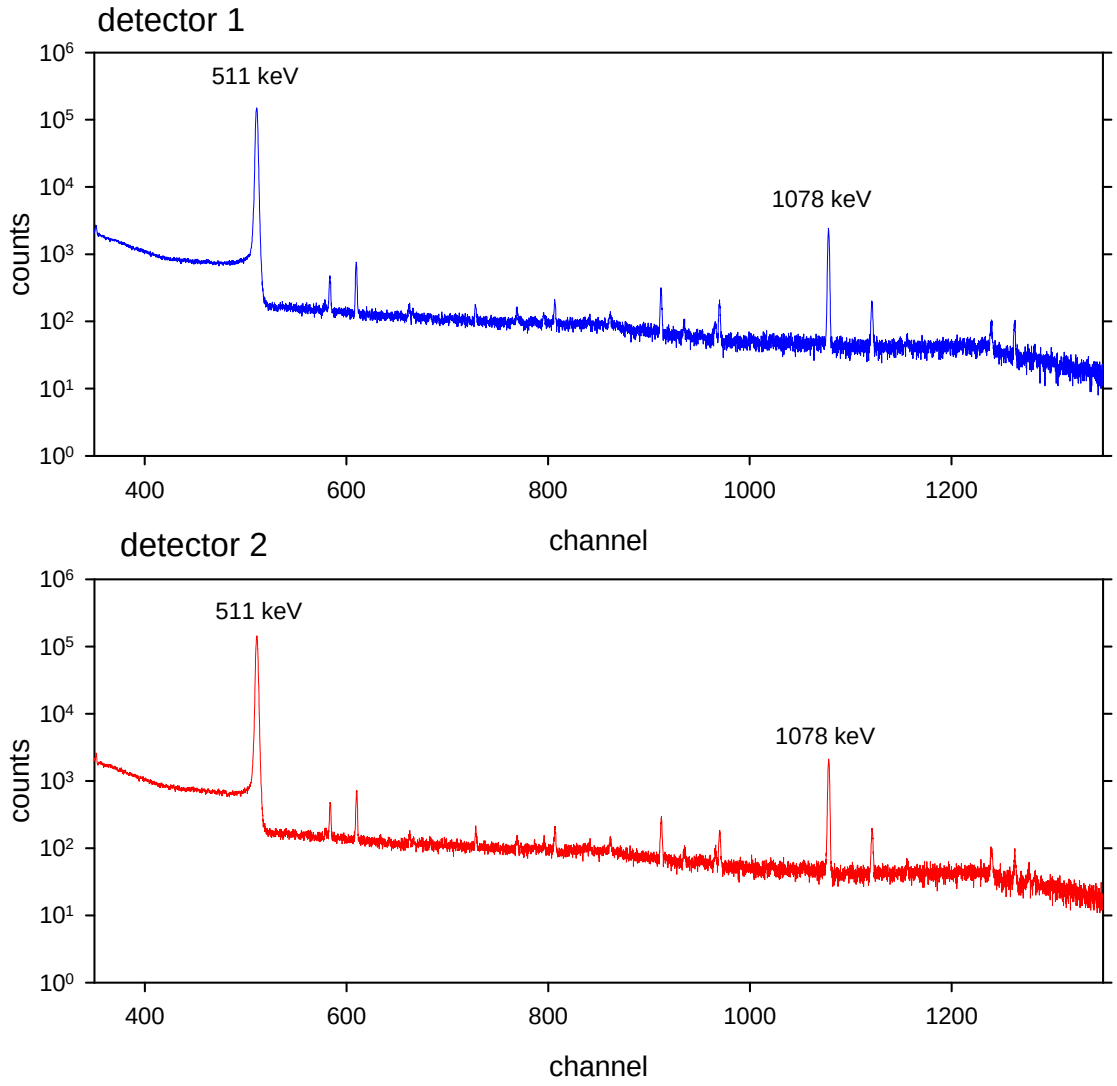

Fig.8 *Calibrated energy spectra for detector 1 and detector 2 taken from file bdif-cal.txt.*

In this mode cmfit performs standard analysis in the same way as in the mode 0 but in addition it reads energy calibration from files `e-cal.txt` (when the entry `calibration = 1`) or `e-cal-smooth.txt` (when the entry `calibration = 2`) created in the raw

analysis mode (mode = 0). Calibrated energy spectrum for the first and the second detector are written in the output file `hist-bdif-cal.txt` and are plotted in Fig. 8.
In addition fine selection of waveforms is performed using digital shape filters created in mode 0 and stored in the file `peakm.txt`. Only the pulses which passed the shape filters are accepted.

6.4. Raw analysis of waveforms measured in coincidence (mode = 2)

Required input files:
`calibration.ini`
`cmfit.ini`
`histograms.ini`
`suffix.ini`
`watchdogs.ini`
calibration files created in mode 0:
`e-cal.txt`
`e-cal-smooth.txt`
file with ideal pulse shapes and shape filters created in mode 0:
`peakm.txt`

Created output files:
histograms:
`hist-bcg_mean.txt`
`hist-bcg_sigma.txt`
`hist-bdif.txt`
`hist-bdif-cal.txt`
`hist-bdif-sess.txt`
`hist-ch_darea.txt`
`hist-ch_wmax.txt`
`hist-chi2sq.txt`
`hist-darea.txt`
`hist-dt.txt`
`hist-reject.txt`
`hist-t.txt`
`hist-warea.txt`
`hist-wmax.txt`
two-dimensional CDB histogram
`ee.txt`
vertical and horizontal cuts from the two-dimensional CDB histogram
`cuts.txt`
binary file with determined energies and times:
`energies-2.dat`

This mode is analogical to mode 0 but is intended for analysis of waveforms measured in coincidence. Hence, the waveforms are analyzed in the same way as in mode 0 and pulses with seriously distorted shape are rejected by the fixed filters. However, additional analysis is performed in mode 2 and two dimensional histograms are created. Determined energy for each waveform and the time interval between the waveforms are written into the output file `energies-2.dat` in binary format. The output file `energies-2.dat` can be read by the program `dcdbt_ee` which enables to create various histograms from these data.

Two-dimensional CDB histogram, i.e. sum of determined energies $E_1 + E_2 - 2m_0c^2$ plotted versus difference of these energies $E_1 - E_2$, is created in mode 2. An example of this two-dimensional histogram stored in the output file `ee.txt` is plotted in Fig. 9. Range of horizontal and vertical axis of this histogram is specified by the entries `RF histogram range (keV)` and `DB histogram range (keV)` in `cmfit.ini`.
Vertical and horizontal cuts from the two-dimensional CDB spectrum are created and written into output file `cuts.txt`. These one dimensional cuts correspond to the resolution function of spectrometer and Doppler broadened annihilation peak and are plotted in Fig. 10.

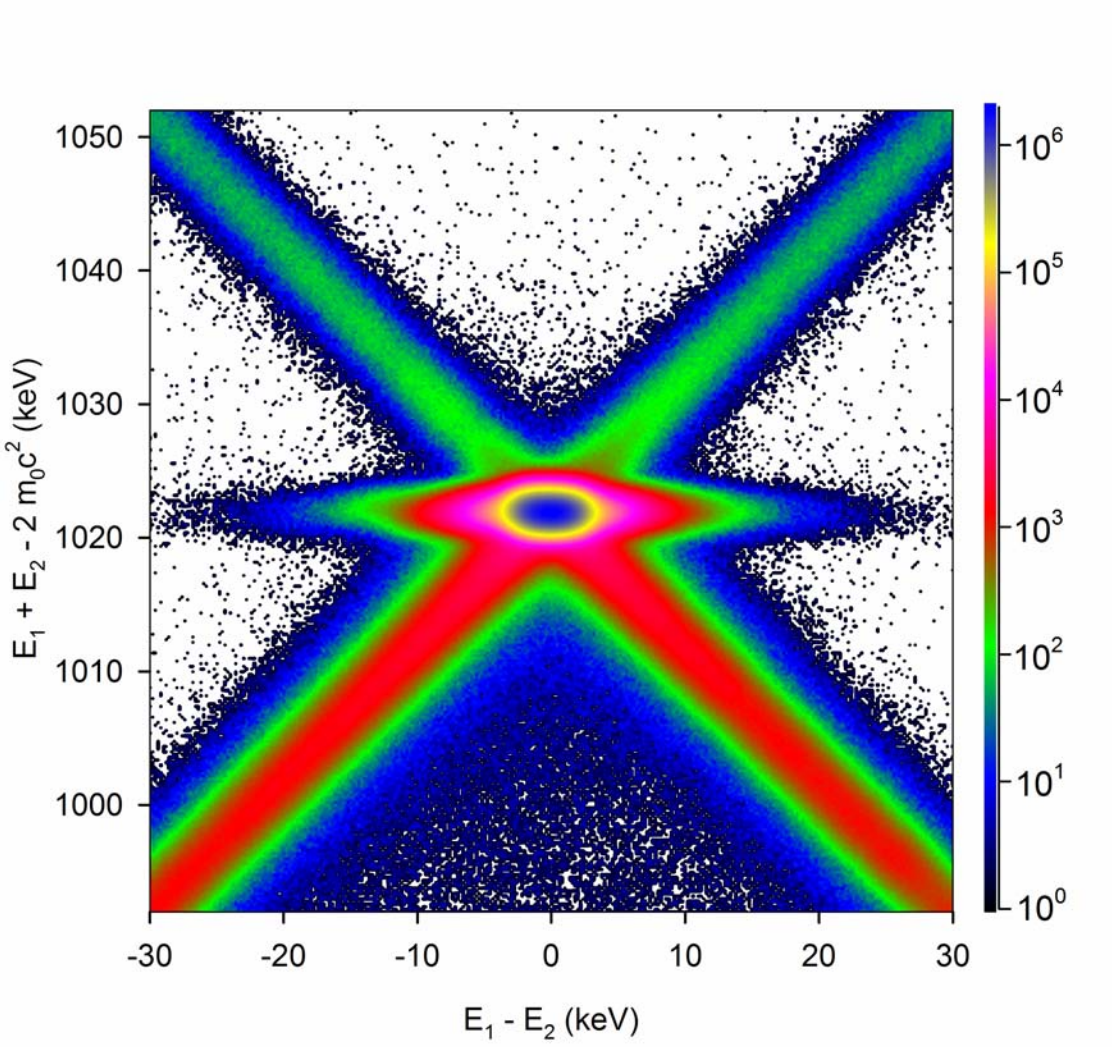

Fig.9 *Two-dimensional CDB energy spectrum created in the mode 2 (output file ee.txt)*

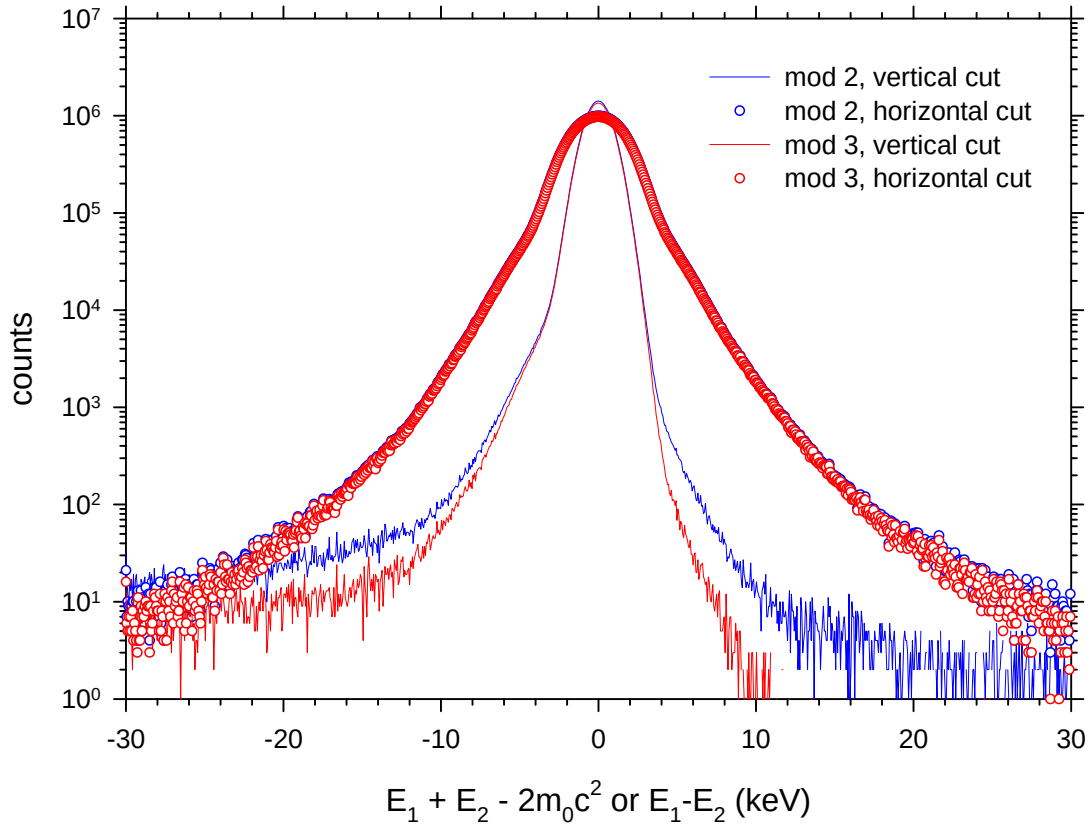

Fig.10 *Vertical and horizontal one-dimensional cuts from the two-dimensional CDB spectrum. The cuts from the two-dimensional CDB spectra obtained in the mode 2 (blue color) are compared with those obtained in the mode 3 (red color). The cuts are stored in the output file cuts.txt.*

6.5. Fine analysis of waveforms measured in coincidence (mode = 3)

Required input files:
`calibration.ini`
`cmfit.ini`
`histograms.ini`
`suffix.ini`
`watchdogs.ini`
calibration files created in mode 0:
`e-cal.txt`
`e-cal-smooth.txt`
file with ideal pulse shapes and shape filters created in mode 0:
`peakm.txt`

Created output files:
histograms:
`hist-bcg_mean.txt`
`hist-bcg_sigma.txt`
`hist-bdif.txt`

`hist-bdif-cal.txt`
`hist-bdif-sess.txt`
`hist-ch_darea.txt`
`hist-ch_wmax.txt`
`hist-chi2sq.txt`
`hist-darea.txt`
`hist-dt.txt`
`hist-reject.txt`
`hist-t.txt`
`hist-warea.txt`
`hist-wmax.txt`
two-dimensional CDB histogram
`ee.txt`
vertical and horizontal cuts from the two-dimensional CDB histogram
`cuts.txt`
binary file with determined energies and times:
`energies-3.dat`

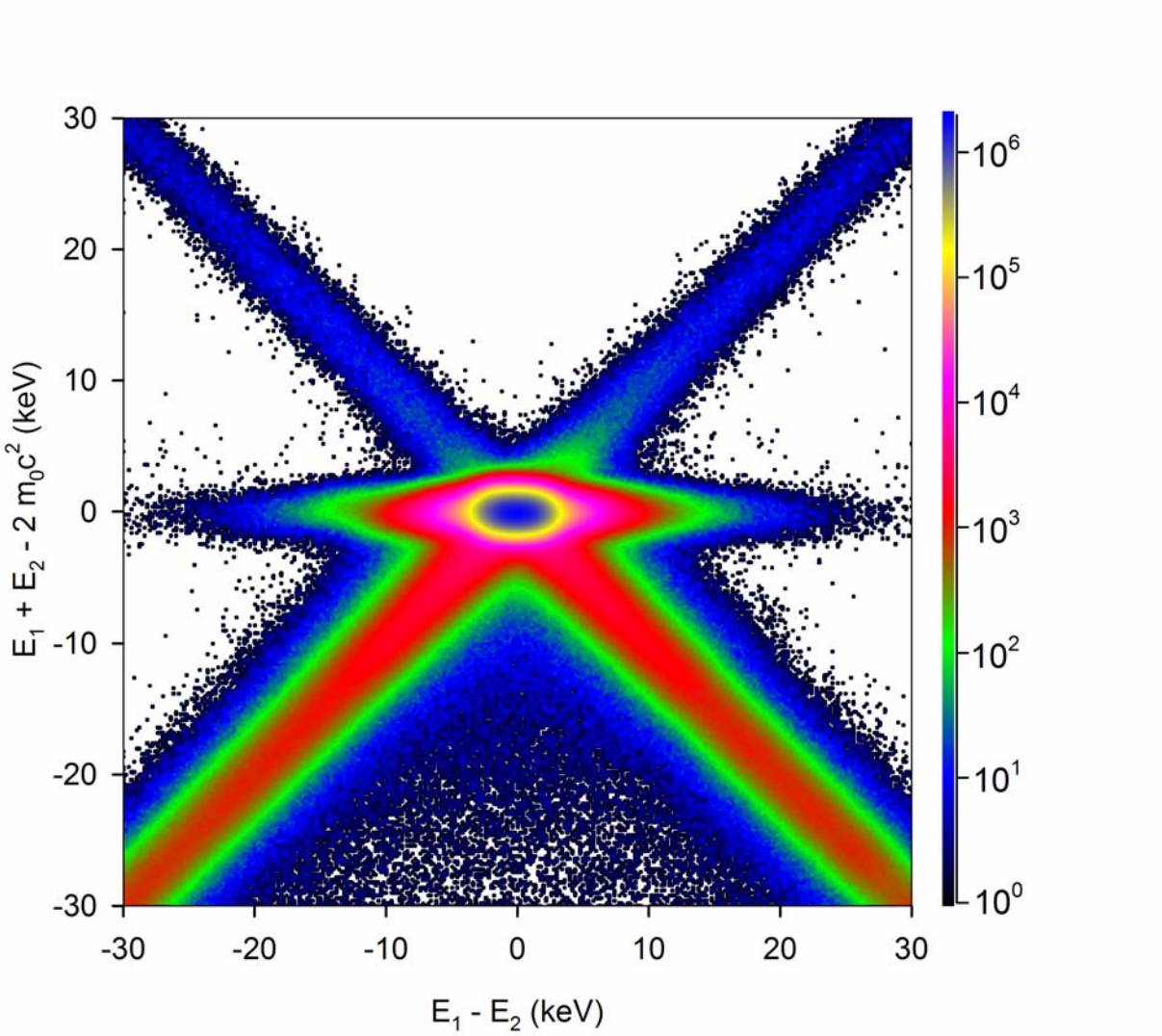

Fig.11 *Two-dimensional CDB energy spectrum created in the mode 3 (output file ee.txt).*

This mode is used for fine analysis of waveforms measured in coincidence. It makes the same analysis of waveforms as mode 2 but in addition the waveforms are inspected by digital shape filters and only waveforms accepted by shape filters are used for creation of histograms and two-dimensional CDB spectra. The determined energies and time interval between waveform registered by the first and the second detector are stored in the binary file `energies-3.dat`. This file can read by the program `dcdbt_ee` which enables to create various histograms specified by user. The two-dimensional CDB energy spectrum created in mode 3 and stored in the file `ee.txt` is plotted in Fig. 11. Vertical and horizontal cuts from the two-dimensional CDB spectrum stored in the output file `cuts.txt` are plotted in Fig. 10 in comparison with the cuts obtained in the mode 2, i.e. without application of shape filters.

References

[1] J. Čížek. M. Vlček, I. Procházka, *Nuclear Instruments and Methods in Physics Research Section A* **623**, 982-994 (2010).

[2] J. Čížek, M. Vlček, F. Lukáč, O. Melikhova, I. Procházka, W. Anwand, M. Butterling, A. Wagner, G. Brauer, *Defect and Diffusion Forum* **331**, 53-73 (2012).

[3] J. Čížek, M. Vlček, I. Procházka, *New Journal of Physics* **14**, 035005 (2012).